Dipole resonances in oxygen isotopes in time-dependent density-matrix theory

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Abstract

The strength functions of isovector dipole resonances in the even oxygen isotopes $^{18\sim24}$O are calculated by using an extended version of the time-dependent Hartree-Fock theory known as the time-dependent density-matrix theory (TDDM). The results are compared with recent experimental data and also with a shell-model calculation. It is found that the observed isotope dependence of low-lying dipole strength is reproduced in TDDM when the strength of the residual interaction is properly chosen. It is also found that there is a difference between the TDDM prediction and the shell-model calculation for ^{24}O.

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The study of structures and reactions of nuclei far from stability has been one of the most active fields of nuclear physics in the past decade [1]. The microscopic description of such nuclei will lead to a better understanding of the interplay among the strong, Coulomb, and the weak interactions as well as the enhanced correlations present in these many-body systems. For neutron rich nuclei, in the extreme limit, the proton and neutron densities may exhibit strikingly different behavior. One of the observables for studying this phenomenon is the evolution of the isovector dipole modes along an isotope chain. Several years ago explorative calculations were performed for isovector dipole ($E1$) and isoscalar quadrupole ($E2$) resonances in the unstable oxygen isotope ^{22}O based on the time-dependent density-matrix theory (TDDM) [2]. It was found that there are low-energy $E1$ and $E2$ modes associated with excess neutrons. At that time there were no experimental data to be compared with and the TDDM calculations were not so quantitative since spin-orbit force was neglected in the calculation of a mean-field potential, and the neutron $2s$ and $1d$ states were assumed to be fractionally occupied, apparently overestimating the effect of ground-state correlations. Recently the isotope dependence of low-lying $E1$ strength has been measured at GSI [3] for oxygen isotopes and compared with a shell-model calculation [4]. The aim of this paper is to present more quantitative calculations of $E1$ modes for these isotopes using the time-dependent Hartree-Fock (TDHF) and the TDDM theories. Two recent improvements make it possible to do better TDDM calculations: one is the treatment of ground-state correlations. As will be described below, an adiabatic treatment of the residual interaction enables us to obtain a correlated ground state which is a stationary solution of TDDM [5]. The other improvement is the extension of the TDDM program so as to include spin-orbit force, as it was done for TDHF calculations [6].

TDDM is an extended version of TDHF and is formulated so as to determine the time evolution of one-body and two-body density matrices ρ and ρ_2 in a self-consistent manner [7]. TDDM, therefore, includes the effects of both a mean-field potential and two-body correlations. The equations of motion for ρ and ρ_2 can be derived by truncating the well-known BBGKY hierarchy for reduced density matrices [8]; To solve the equations of motion for ρ and ρ_2, we expand ρ and C_2 using a finite number of single-particle states ψ_α which satisfy a TDHF-like equation,

$$\rho(11',t) = \sum_{\alpha\alpha'} n_{\alpha\alpha'}(t)\psi_\alpha(1,t)\psi^*_{\alpha'}(1',t), \tag{1}$$

$$\begin{aligned} C_2(121'2',t) &= \rho_2 - A(\rho\rho) \\ &= \sum_{\alpha\beta\alpha'\beta'} C_{\alpha\beta\alpha'\beta'}(t) \\ &\quad \times \psi_\alpha(1,t)\psi_\beta(2,t)\psi^*_{\alpha'}(1',t)\psi^*_{\beta'}(2',t), \end{aligned} \tag{2}$$

where the numbers denote space, spin and isospin coordinates. Thus the equations of motion of TDDM consist of the following three coupled equations [7]:

$$i\hbar\frac{\partial}{\partial t}\psi_\alpha(1,t) = h(1,t)\psi_\alpha(1,t), \tag{3}$$

$$i\hbar\dot{n}_{\alpha\alpha'} = \sum_{\beta\gamma\delta}[\langle\alpha\beta|v|\gamma\delta\rangle C_{\gamma\delta\alpha'\beta} - C_{\alpha\beta\gamma\delta}\langle\gamma\delta|v|\alpha'\beta\rangle], \tag{4}$$

$$i\hbar\dot{C}_{\alpha\beta\alpha'\beta'} = B_{\alpha\beta\alpha'\beta'} + P_{\alpha\beta\alpha'\beta'} + H_{\alpha\beta\alpha'\beta'}, \tag{5}$$

where h is the mean-field Hamiltonian and v the residual interaction. The terms on the right-hand side of Eq.(5) contain all the two-body correlations including those induced by the Pauli exclusion principle [2]. The TDDM equations of motion satisfy conservation laws of the total number of particles and the total momentum and energy. The small amplitude limit of TDDM was investigated [9] and it is found that, if only the 1 particle - 1 hole and 1 hole - 1 particle elements of $n_{\alpha\alpha'}$ and the 2 particle - 2 hole and 2 hole - 2 particle elements of $C_{\alpha\beta\alpha'\beta'}$ are taken, the small amplitude limit of TDDM is equivalent to the conventional second RPA (SRPA) [10]. Thus TDDM is more general framework than the conventional SRPA.

The $E1$ strength function is calculated according to the following three steps:

1) A static Hartree-Fock (HF) calculation is performed to obtain the initial ground state. The Skyrme III with spin-orbit force is used as the effective interaction. It has been reported [11] that the Skyrme III is useful even for very neutron rich nuclei. Unoccupied single-particle states up to the $2s$ and $1d$ orbits are also calculated for both protons and neutrons to solve the TDDM equations for $n_{\alpha\alpha'}$ and $C_{\alpha\beta\alpha'\beta'}$. The single-particle wavefunctions are confined to a cylinder with length 20fm and radius 10fm. (Axial symmetry is imposed to calculate the single-particle wavefunctions [6].) The mesh size used is 0.5fm. The neutron $1d_{5/2}$ state is assumed partially occupied to obtain the HF ground states for ^{18}O and ^{20}O.

2) To obtain a correlated ground state, we evolve the HF ground state using the TDDM equations and the following time-dependent residual interaction of the δ-function form

$$v(t) = v_0(1 - e^{-t/\tau})\delta^3(\vec{r} - \vec{r'}). \tag{6}$$

The time constant τ should be sufficiently large to obtain a nearly stationary solution of the TDDM equations [5]. We choose τ to be 150fm/c. The strength of the residual interaction is determined to approximately reproduce the observed occupation probability of the proton $1d_{5/2}$ state in ^{16}O [12]. The obtained value of v_0 is -230MeVfm^3, which might be smaller than the value of around -300MeVfm^3 found in the literature for pairing-gap calculations [13]. The time step size used to solve the TDDM equations is 0.75fm/c. The calculated occupation probabilities of the neutron $2s_{1/2}$ and $1d_{3/2}$ are $2 \sim 3\%$ in the oxygen isotopes considered here.

3) The $E1$ mode is excited by boosting the single-particle wavefunctions at $t = 5\tau$ with the dipole velocity field:

$$\psi_\alpha(5\tau) \longrightarrow e^{ikD(z)}\psi_\alpha, \tag{7}$$

where

$$D(z) = \frac{N}{A}z, \quad (-\frac{Z}{A}z) \ \text{ for protons (for neutrons).} \tag{8}$$

Here Z are N are the numbers of protons and neutrons, respectively, and $A = Z + N$. When the boosting parameter k is sufficiently small, the strength function defined by

$$S(E) = \sum_n |\langle\Phi_n|\hat{D}|\Phi_0\rangle|^2\delta(E - E_n) \tag{9}$$

is obtained from the Fourier transformation of the time-dependent dipole moment $D(t)$ as

$$S(E) = \frac{1}{\pi k\hbar}\int_0^\infty D(t)\sin\frac{Et}{\hbar}dt, \tag{10}$$

where

$$D(t) = \int D(z)\rho(\vec{r},t)d^3\vec{r}. \tag{11}$$

In Eq.(9) $|\Phi_0\rangle$ is the total ground-state wavefunction and $|\Phi_n\rangle$ the wavefunction for an excited state with excitation energy E_n. It is very time consuming to solve the TDDM equations (especially Eq.(5)) for a long period. So we stop TDDM calculations at $t = 1200$fm/c. Therefore, the upper limit of the time integration in Eq.(10) is limited to 450fm/c. To reduce fluctuations in $S(E)$, the dipole moment is multiplied by a damping factor $e^{-\Gamma t/2\hbar}$ with $\Gamma = 1$MeV before the time integration. Since the integration time is limited, the strength function in a very low energy region ($E < 2\pi\hbar/450 \approx 3$MeV) is not well determined. The energy-weighted sum rule (EWSR) is expressed as

$$\begin{aligned}\int S(E)EdE &= \frac{1}{2}\langle\Phi_0|[\hat{D},[H,\hat{D}]]|\Phi_0\rangle \\ &= \frac{\hbar^2}{2m}\frac{ZN}{A} \\ +\frac{t_1+t_2}{4}(\int \rho_p(\vec{r})\rho_n(\vec{r})d^3\vec{r} &+ \sum_{\alpha\alpha'\in p,\beta\beta'\in n}\int \psi^*_\alpha(\vec{r})\psi^*_\beta(\vec{r})\psi_{\alpha'}(\vec{r})\psi_{\beta'}(\vec{r})d^3\vec{r}C_{\alpha'\beta'\alpha\beta}),\end{aligned} \tag{12}$$

where m is the nucleon mass, and t_1 and t_2 are the parameters for the momentum dependent parts of the Skyrme interaction. We assume that the Hamiltonian H consists of a two-body interaction of the Skyrme type. The first term on the right-hand side of the above equation corresponds to the classical Thomas-Reiche-Kuhn (TRK) sum rule and the second term the enhancement term due to the momentum dependence of the Hamiltonian. The contribution of the momentum dependent part is about 28% of the total EWSR value in the oxygen isotopes considered here and the term proportional to $C_{\alpha\beta\alpha'\beta'}$ describing the effects of ground-state correlations is quite small (less than 1% of the total sum rule value).

In Figs.1$\sim$4 the $E1$ strength functions of $^{18\sim24}$O calculated in TDDM (solid line) are compared with those in TDHF (dotted line). The TDHF calculations presented here are equivalent to the RPA calculations without any truncation of unoccupied single-particles states because the TDHF equation for the boosted single-particle wavefunctions ψ_α is solved in coordinate space. The boundary condition for the continuum states, however, is not properly taken into account in our calculation because all the single-particle wave functions are confined to the cylinder. Therefore, the calculated strength functions slightly depend on the cylinder size. The difference between the TDDM and TDHF calculations is due to the effect of two-body correlations, which has two aspects: one is to induce ground-state correlations which increase the occupation probabilities of weakly-bound neutron orbits. The increase in low-lying strength ($E < 15$MeV) seen in the TDDM results for all the isotopes is due to partial occupation of the neutron $2s_{1/2}$ and $1d_{3/2}$ states. The comparison between the TDDM result for ^{24}O and those for other isotopes suggests that the occupation of the neutron $2s_{1/2}$ state is responsible for the increase in the $E1$ strength in the very

low energy region (around $E = 5$MeV). This is because the appearance of the prominent peak at 6MeV in ^{24}O is related to nearly full occupation of the neutron $2s_{1/2}$ state. The other aspect of two-body correlations is to increase the width of the giant dipole resonance (GDR) which is located around 25MeV. There are background 2 particle - 2 hole states which consist of $1\hbar\omega$ excitations of protons and $0\hbar\omega$ excitations of neutrons. The coupling of the GDR to these states gives the spreading of the GDR strength. The fractions of the EWSR values depleted in the energy range between 0MeV to 40MeV are about 85% in TDDM and about 90% in TDHF. The EWSR values depleted below 15MeV are shown in Fig.5. The ordinate indicates the ratio of the EWSR value to the TRK value. The results in TDDM with $v_0 = -230$MeVfm^3 (rhombus) are smaller than the experimental data except for ^{22}O. In TDDM the EWSR values in the low-energy region crucially depend on the strength of the residual interaction. Since the strength of the residual interaction is not well-known in unstable nuclei, we made TDDM calculations using slightly stronger residual interaction with $v_0 = -330$MeVfm^3 to increase $E1$ strength in low-energy region. The value of $v_0 = -330$MeVfm^3 was used in our previous studies [2,14] and found to give reasonable spreading widths for giant resonances in stable nuclei [14]. As an example of the TDDM calculations with $v_0 = -330$MeVfm^3, we show the result for ^{20}O in Fig.6. The increase in the strength below 10MeV is due to the increase in the occupation probability of the neutron $2s_{1/2}$ state and the enhancement of the peak at 15MeV is caused by further fragmentation of the GDR strength. The EWSR values depleted below 15MeV are shown by circles in Fig.5. The magnitude of the low-lying strength is increased and now becomes close to the experimental data except for ^{22}O. The fact that the low-lying $E1$ strength in ^{20}O is most increased with the use of the stronger residual interaction may be explained by the large fragmentation of the GDR strength as seen in Fig.6. The TDDM results for ^{24}O shown in Fig.5 significantly differ from the shell-model calculation [4]. The difference originates in the fact that the shell-model calculation gives much smaller spreading width to the GDR in ^{24}O than the TDDM and TDHF calculations do. Since the large amount of the $E1$ strength is concentrated in the GDR, the low-lying $E1$ strength calculated in the shell model becomes small in ^{24}O.

In summary, the strength functions of the isovector dipole resonances in the even oxygen isotopes $^{18\sim24}$O were calculated by using an extended version of TDHF known as TDDM. These calculations are much more improved and quantitative than the previous ones [2] in two aspects: the inclusion of spin-orbit force in a mean-field potential and the use of a correlated ground state. The results were compared with recent experimental data and also with a shell-model calculation. It was found that, if the strength of the residual interaction is properly chosen, TDDM approximately reproduces the observed low-lying $E1$ strength. It was also found that the TDDM prediction differs from the shell-model calculation for ^{24}O. It was discussed that this originates in the difference in the spreading width of the GDR between the two models.

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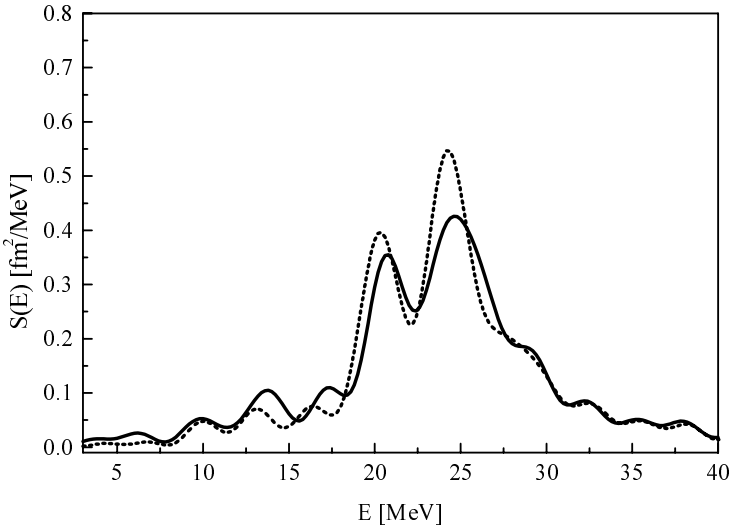

FIG. 1. Strength functions of isovector dipole resonances in ^{18}O calculated in TDDM (solid line) and in TDHF (dotted line).

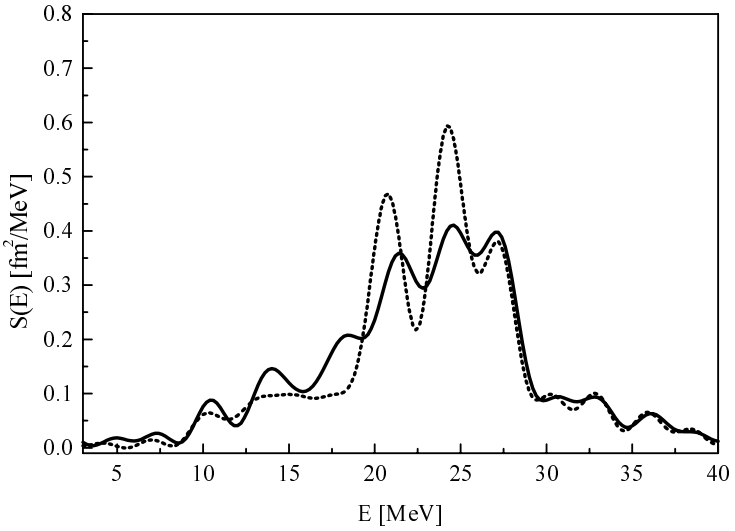

FIG. 2. Strength functions of isovector dipole resonances in ^{20}O calculated in TDDM (solid line) and in TDHF (dotted line).

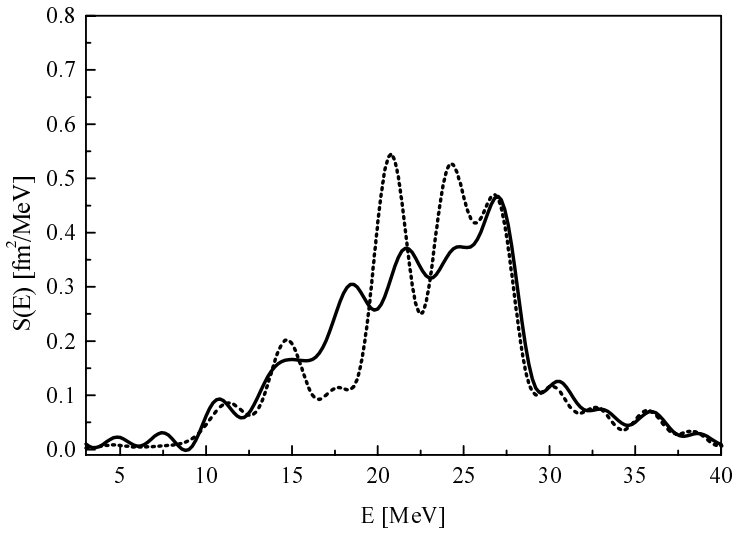

FIG. 3. Strength functions of isovector dipole resonances in ^{22}O calculated in TDDM (solid line) and in TDHF (dotted line).

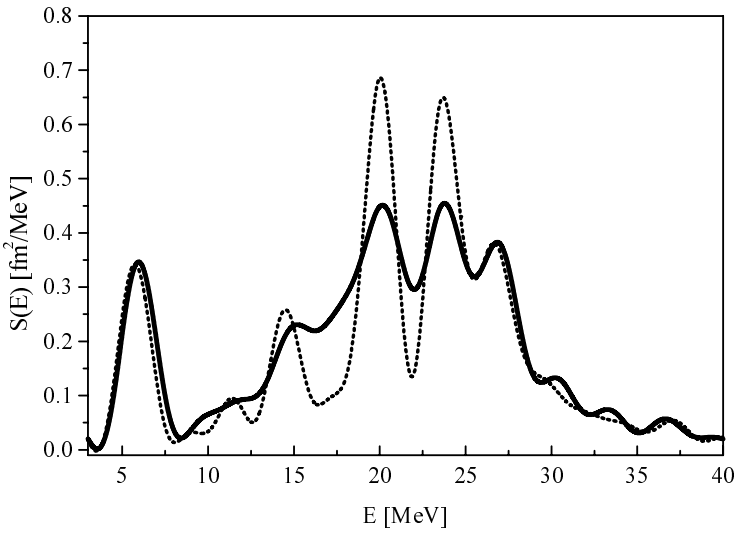

FIG. 4. Strength functions of isovector dipole resonances in ^{24}O calculated in TDDM (solid line) and in TDHF (dotted line).

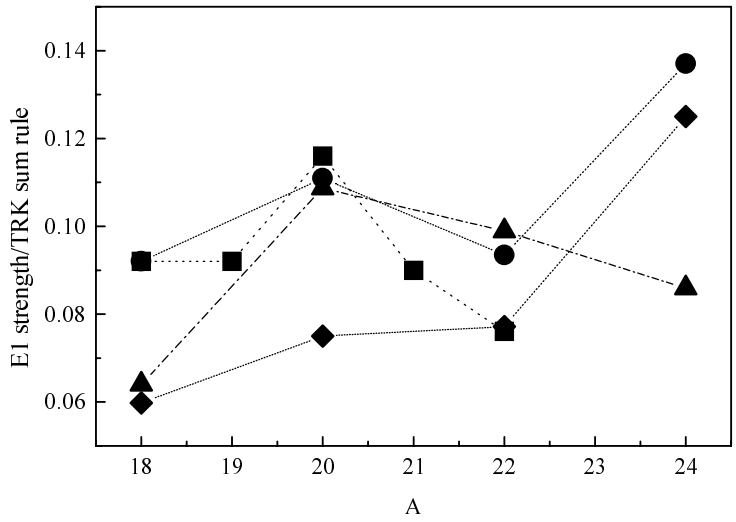

FIG. 5. Isotope dependence of the low-lying $E1$ strength. The square, triangle, rhombus, and circle indicate the experiment[2)], the shell-model calculation[3)], the TDDM results with $v_0 = -230\text{MeVfm}^3$ and -330MeVfm^3, respectively.

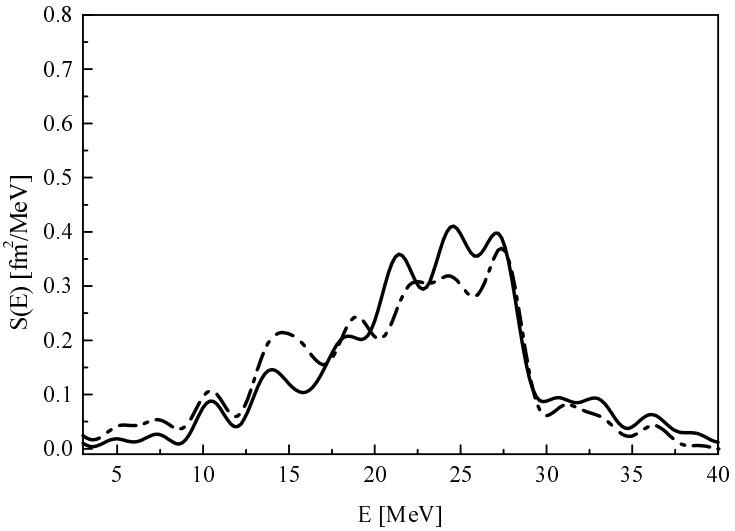

FIG. 6. Strength functions of isovector dipole resonances in ^{20}O calculated with $v_0 = -230\text{MeVfm}^3$ (solid line) and with $v_0 = -330\text{MeVfm}^3$ (dot-dashed line).